11-1964

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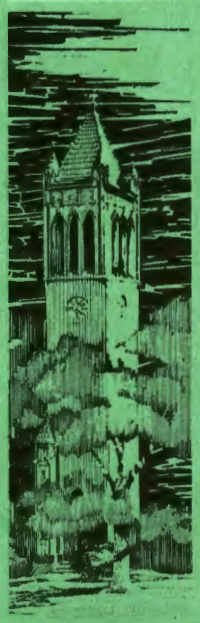
Disciplines
Chemistry | Computer Sciences

IS-1042



IOWA STATE UNIVERSITY

PACK2, A FORTRAN CRYSTALLOGRAPHIC MOLECULAR PACKING PROGRAM

by

Donald E. Williams

AMES LABORATORY

RESEARCH AND DEVELOPMENT REPORT

U.S.A.E.C.

IS-1042

Chemistry (UC-4)
TID 4500, October 1, 1964

UNITED STATES ATOMIC ENERGY COMMISSION

Research and Development Report

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by

Donald E. Williams

November, 1964

Ames Laboratory
at
Iowa State University of Science and Technology
F. H. Spedding, Director
Contract W-7405 eng-82

This report is distributed according to the category Chemistry (UC-4), as listed in TID-4500, October 1, 1964.

Printed in USA. Price $ 2.00 Available from the

Office of Technical Services
U. S. Department of Commerce
Washington 25, D. C.

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Donald E. Williams

ABSTRACT

This report describes a computer program which performs an analysis of molecular packing in crystals. All space group symmetries are allowed. The packing energy of a molecular crystal structure, known or proposed, may be evaluated using appropriate nonbonded interatomic potential functions.

For unknown crystal structures, the program may be used to assist the solution of the diffraction phase problem. In this application the program minimizes the packing energy for a molecule of assumed dimensions by a steepest descent method. The adjustable parameters are the molecular translations and rotations, specified internal molecular rotations (subrotations), and the lattice constants.

The program may also be used to study nonbonded interatomic potential functions. These functions can be evaluated by a comparison of the calculated parameters found by the program with the observed parameters for known crystal structures.

INTRODUCTION

The availability of fast digital computers has made possible a more detailed analysis of the packing structure of molecular crystals. Much useful information may be derived from such an analysis. The parameters for nonbonded interatomic potential functions may be checked and improved by analysis of known crystal structures. Thermodynamic quantities for molecular crystals may also be calculated. Examples of such thermodynamic quantities are the heat of sublimation and the energy barrier to molecular rotation in the crystal. Furthermore, the

packing energies and lattice constants for hypothetical structures of different symmetry may be calculated and compared with the known structure.

A second important type of application of packing analysis is to assist in the solution of the diffraction phase problem for unknown crystal structures. If the molecule is of known dimensions, or a reasonable molecular model can be postulated, a possible position of the molecule in the unit cell of known size and symmetry can be found. If the molecule is completely rigid, and is in a general crystallographic position, three rotational and three translational coordinates specify its position. Intramolecular flexibility can be introduced by allowing internal rotation (subrotation) around selected bonds within the molecule. Thus the rotational orientation of a phenyl substituent on a molecule, for example, can be treated as a parameter. The crystal structure found by packing analysis can be quickly checked for rough agreement with diffraction data. The correct packing model can then be refined by means of rigid body structure factor least squares or by the Fourier electron density method.

MATHEMATICAL METHOD

The packing energy of the crystal, E, is defined in the program as the sum of all potential energies of nonbonded atomic interactions. Pairwise additivity of the interatomic potentials is assumed, and zero point energy and rotational energy are neglected. Thus, if the potential energy of interaction between atom j in a given molecule and atom k in

some surrounding molecule is E_{jk}, then

$$E = \tfrac{1}{2} \Sigma E_{jk}$$

where the sum is taken over all of the neighbors of a given molecule.

The nonbonded interatomic potential functions are defined in the subroutine EJKL. In this subroutine, four parameters may be used for each type of interatomic potential. This subroutine may be readily altered by the user; the original program uses the Buckingham formula

$$E_{jk} = -Ad_{jk}^{-6} + B \exp(-d_{jk}/\rho) .$$

For convenience this formula is rewritten as

$$E_{jk} = \left[E_{jk}^{o}/(1 - 6\rho/d_{jk}^{o}) \right] \left[d_{jk}^{-6} d_{jk}^{o\,6} - (6\rho/d_{jk}^{o}) \exp(d_{jk}^{o} - d_{jk})/\rho) \right] ,$$

where E_{jk}^{o} is the potential energy at the minimum, and d_{jk}^{o} is the interatomic distance at the minimum potential. The relations between E_{jk}^{o} and d_{jk}^{o} and the coefficients of the original equation are

$$E_{jk}^{o} = -Ad_{jk}^{o\,-6}(1 - 6\rho/d_{jk}^{o})$$

$$d_{jk}^{o\,7} = (6\rho A/B) \exp(d_{jk}^{o}/\rho) .$$

INTERATOMIC DISTANCES

We now wish to express the nonbonded distances d_{jk} as a function of the crystal packing structure, with reference to rotation and translation of the molecule in the unit cell, subrotations around bonds within

the molecule, and the lattice constants.

The reference molecule (unit cell fractional coordinates x_j) is surrounded by symmetry related molecules with coordinates x_{kn}, where the first subscript refers to the kth atom in the molecule and the second subscript refers to the translation and symmetry operation necessary to obtain the nth symmetry related molecule. Thus we have the equation

$$x_{kn} = t_n + s_n x_k ,$$

where x_{kn}, t_n, and x_k are column 3-vectors, and s_n is a 3x3 matrix. If we define the 3x3 matrix D which transforms unit cell space into a cartesian reference system, we have in the cartesian system

$$X_{kn} = T_n + S_n X_k ,$$

where $X_k = Dx_k$, $T_n = Dt_n$, and $S_n = Ds_nD^{-1}$. The nonbonded interatomic distance is

$$d_{jkn} = |X_j - X_{kn}|$$

for the atomic positions of the trial model being considered.

The effect of a small rotation, centered at X_θ^o, on the reference molecule is given by the equation

$$X_j' = R_\theta(X_j - X_\theta^o) + X_\theta^o, \qquad R_\theta = \begin{pmatrix} 1 & -\theta_3 & \theta_2 \\ \theta_3 & 1 & -\theta_1 \\ -\theta_2 & \theta_1 & 1 \end{pmatrix} .$$

The effect of the rotation on a symmetry related atom is given by

$$X'_{kn} = T_n + S_n\left[R_\theta(X_k - X^o_\theta) + X^o_\theta\right] .$$

The R_θ matrix is orthonormalized by the program before it is actually used to obtain the new molecular position. The effect of a small translation U is

$$X'_j = X_j + U , \qquad X'_{kn} = T_n + S_n(X_k + U) .$$

The effect of a small subrotation R_ψ around a bond in the molecule is given by

$$X'_j = R_\psi(X_j - X^o_\psi) + X^o_\psi ,$$

where the transformation is applied only to atoms in the rotating group. The center of subrotation, X^o_ψ, may be taken as one of the bond atom positions. The matrix R_ψ may be formed by finding the matrix C which transforms cartesian space such that the first axis is parallel to the bond direction. We then have

$$R_\psi = C^{-1}PC , \qquad P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\psi & -\sin\psi \\ 0 & \sin\psi & \cos\psi \end{pmatrix} .$$

The effect of the subrotation on symmetry related molecules may be found analogously to the θ rotations.

The effect of a small change in the lattice constants is to change the D matrix to D':

$$X'_j = D'D^{-1}X_j , \qquad X'_{kn} = D'D^{-1}T_n + D'D^{-1}S_n D(D')^{-1}X_k .$$

STEEPEST DESCENT PROCEDURE

The derivative of E with respect to the parameter p_m is evaluated numerically in the program by incrementing p_m and recalculating E. Thus

$$\frac{\partial E}{\partial p_m} = \frac{E' - E}{\epsilon_m} ,$$

where E' is the new value of E found after incrementing the parameter p_m by the amount ϵ_m.

The direction of most rapid change in E is along the gradient vector. To minimize E we move along the gradient by an amount λ to find the parameter shifts Δp_m:

$$\Delta p_m = -\lambda \frac{\partial E}{\partial p_m} .$$

By applying the shifts Δp_m we arrive at a new value of E:

$$E' = E + \sum_m \Delta p_m \frac{\partial E}{\partial p_m} = E - \lambda \sum_m \left(\frac{\partial E}{\partial p_m} \right)^2 .$$

Thus the value of λ may be found by estimation of the excess packing energy, $\Delta E = E - E'$, of the current model:

$$\lambda = \Delta E / \sum_m \left(\frac{\partial E}{\partial p_m} \right)^2 .$$

The program uses a binary chopping technique to reduce the estimated value of ΔE as the problem converges. A parameter overshoot condition is detected by the program if the current parameter shifts cause the calculated packing energy to increase. When this occurs, ΔE is halved and the problem recycled using half shifts. This process can be repeated several times if necessary.

CLOSE NONBONDED APPROACH TABLE

Since the number of atom pair combinations in a typical unit cell of an organic crystal is quite large, ways must be found to reduce the number of symmetry interactions to be considered. It does not matter that most of these distances can quickly be rejected as too long to be of interest once calculated; we do not wish to calculate the uninteresting distances in the first place.

The number of symmetry-cell translation combinations to be considered can quickly be reduced in the following way. We wish to sum all distances up to $d^o_{jk} + \Delta d$. If d^o_{max} is the maximum d^o_{jk} in the potential parameter list, a radius $r = (d^o_{max} + \Delta d)/2$ about the atoms of the reference molecule needs to be considered. A box with edges parallel to the cartesian axes enclosing the reference molecule with a minimum clearance of r at each face can be constructed. This box may now be symmetry and cell translation transformed. Only those symmetry-cell translation combinations which yield overlapping boxes need to be considered.

A large search still remains, that of sorting through the remaining

symmetry combinations. This can be done on a high speed computer, but preferably not for each steepest descent cycle, because of the time required. We anticipate that the shifts Δp_m will be small, so that a table may be stored in the memory of the computer which gives the atom pairs that are sufficiently close to be considered. This table may be used for several rapid cycles of refinement, until the molecule shifts by a sufficient amount so as to require calculation of a new table. In the original program this table has a maximum of 1800 entries.

MISCELLANEOUS PROGRAM DETAILS

Method of Reference to Potential Functions

Each atom J in the molecule is assigned a reference number IPOTR(J). A reference table IPRET(M, N), where M = IPOTR(J) and N = IPOTR(K), contains an integer IP referencing a set of potential parameters contained in the parameter list.

In summing the interatomic potentials E_{jk}, the program does not apply the factor $\frac{1}{2}$ to the sum, E. Thus each interatomic potential must be multiplied by $\frac{1}{2}$ to put E on an absolute scale. If the interatomic potentials are on an absolute scale, the program calculates and minimizes 2E.

Specification of Symmetry Operations

The program is so arranged that the first symmetry operation must specify the basic molecule, i. e., coordinates x, y, z with no translation. This restriction simplifies the handling of subrotations in making up

the close nonbonded approach table.

Specification of Subrotations

Each atom J in the molecule is assigned a reference number IPSI(J). Intramolecular subrotation interactions are evaluated only for different nonzero values of IPSI(J). In other words, interactions between atoms having the same value of IPSI(J) or if one or both of the atoms has IPSI(J) equal to zero are not considered. Thus the atoms defining the bond about which subrotation occurs will normally be assigned zero IPSI(J) values. A dummy nonzero IPSI(J) value may be assigned to appropriate nonsubrotating group atoms. An example of IPSI(J) assignments is shown in Fig. 1.

Dependent Parameters

User's subroutine PATCH(PARW) is called to set any dependent parameters. This subroutine is called when the parameters are incremented in the derivative section, and again when the steepest descent shifts are obtained. The unselected parameters in the list PARW should be set according to the dependent relationship desired. For example, suppose it is desired that subrotation 2 be equal and opposite in sign to subrotation 1. Then the appropriate Fortran statement in subroutine PATCH is PARW(14) = -PARW(13). The sequence of the parameters in the list PARW is explained in the program Fortran listing.

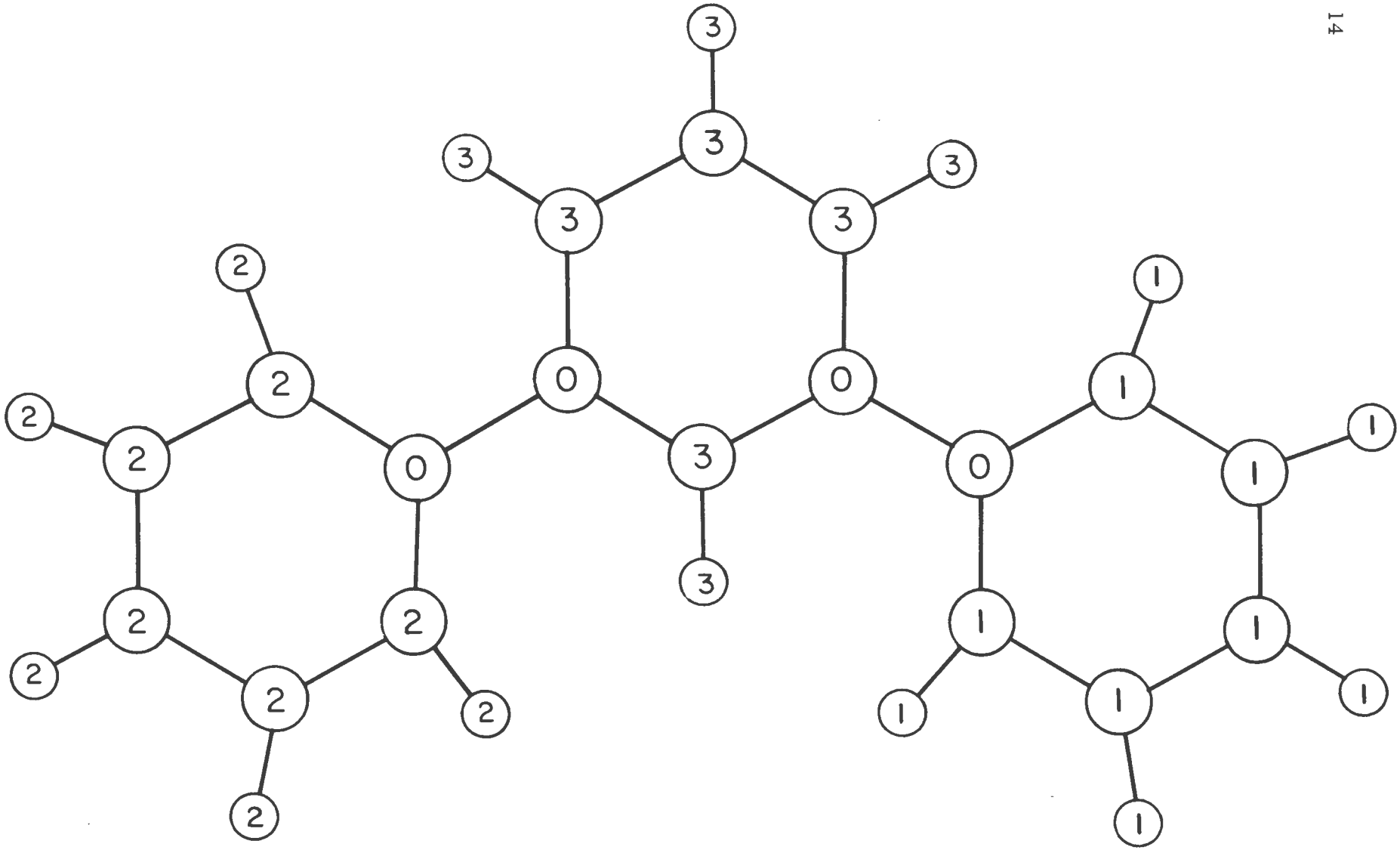

Fig. 1. An example of IPSI(J) assignments for 1, 3-diphenylbenzene. Subrotations 1 and 2 may be varied. Dummy subrotation 3 is not varied and serves to include the appropriate intramolecular energy terms in the calculation.

Output Routine

The program normally outputs a list of all input information, information about the makeup of the close nonbonded approach table, and the parameter shifts and packing energy for each steepest descent cycle. The user may alter subroutine OUTPT to output any additional printed information and punched cards desired. This subroutine is called after the NC cycles have been completed. The original routine shown in the Fortran listing outputs the STWE table, a list of distances which are shorter than the distance at the potential minimum by a specified amount, parameter cards for recycling the program, and input cards for a structure factor least squares program. All information in common storage is available to this subroutine.

SYMBOLIC PROGRAM LISTING

```
      START     ACCNTACC15  @D.WILLIAMS@                                    PCGC
      COMPILE   RUN  FORTRAN LIST                                           PCGC
C      PACK2  CRYSTALLOGRAPHIC PACKING PROGRAM  D.WILLIAMS  AUG.1964
C
C      INPUT TO PROGRAM
C
C      1. TAPE ASSIGNMENT CARD  FORMAT(7(8X,I2))
C          COL. 9-10       NINP       INPUT TAPE NO.
C          COL.19-20       NOUT       OUTPUT TAPE NO.
C          COL.29-30       KEY        +1 TO TERMINATE PROGRAM, OR BLANK
C      2. TITLE CARD  FORMAT(14A5,A2)
C          COL. 1-72       TITLE
C      3. CONTROL CARD  FORMAT (8I5,F10.4)
C          COL. 1- 5       NS         NUMBER OF SYMMETRY CARDS
C          COL  6-10       NA         NUMBER OF ATOMS IN ASYMMETRIC UNIT
C          COL.11-15       NTHE       NUMBER OF RIGID BODIES
C          COL.16-20       NPSI       NUMBER OF SUBROTATIONS (ZERO OK)
C          COL.21-25       NPOT       NO. SETS OF POTENTIAL PARAMETERS
C          COL.26-30       NPRET      WORKING DIMENSION OF IPRET TABLE
C          COL.31-35       INCEL      +1 IF CELL TO CARTESIAN TRANSFORM-
C                                       ATION IS NEEDED, OR BLANK
C          COL.36-40       NC         NUMBER OF REFINEMENT CYCLES DESIRED
C          COL.41-50       DELTE      ESTIMATE OF E(MODEL)-E(FINAL)
C      4.  INITIAL ROTATION MATRIX  FORMAT(9F8.2)
C          COL. 1- 8       RMINP(1,1,1)   RIGID BODY 1
C          COL. 9-16       RMINP(1,2,1)
C          ...
C          COL.65-72       RMINP(3,3,1)
C      5.  ROTATIONAL CENTER AND INITIAL TRANSLATION CARD  FORMAT(6F10.2)
C          COL. 1-10       XZTHE(1,1)     RIGID BODY 1
C          ...
C          COL.51-60       XTRAN(3,1)
C      6.  INITIAL ROTATION MATRIX  FORMAT(9F8.2)  FOR RIGID BODY 2
C                                       READ ONLY IF NTHE=2
C      7.  ROTATIONAL CENTER AND INITIAL TRANSLATION CARD  FORMAT(6F10.2)
C                                       FOR RIGID BODY 2, READ IF NTHE=2
C      8.  LATTICE CONSTANT CARD  FORMAT(6F10.4)
C          COL. 1-10       A          ANGSTROMS
C          ...
C          COL.51-60       GAMMA      DEGREES
C      9.  POTENTIAL PARAMETER CARDS  FORMAT(4F10.5,32X)  NO.=NPOT
C          COL. 1-10       EOJK/2.0   KILOCALORIES/MOLE
C          COL.11-20       DOJK       ANGSTROMS
C          COL.21-30       RHOJK      ANGSTROMS(-1)
C          COL 31-40       MJK        EXPONENT
C     10.  SYMMETRY CARDS  FORMAT(3F10.8,9F4.0,6X)  NO.=NS
C          FIRST SYMMETRY CARD SPECIFIES THE BASIC MOLECULE - I.E.,
C            XYZ WITH NO TRANSLATION
C          COL. 1-10       ST(1,J)    TRANSLATION SYMMETRY IN X
C          ...
C          COL.31-34       SS(1,1,J) SYMMETRY MATRIX ELEMENT
C          COL.35-38       SS(1,2,J)
C          ...
C          COL.63-66       SS(3,3,J)
C     11.  ATOMIC PARAMETER CARDS  FORMAT(3F10.8,3I10,12X)  NO.=NA
C          COL. 1-10       XC(1,J)  EITHER CELL OR CARTESIAN DEPENDING
C          COL.11-20       XC(2,J)    ON INCEL VALUE
C          COL.21-30       XC(3,J)
C          COL.31-40       ITHE(J)   RIGID BODY GROUP NUMBER
C          COL.41-50       IPSI(J)  SUBROTATION GROUP NUMBER (ZERO OK)
```

```
C          COL.51-60      IPOTR(J) REFERENCE TO IPRET TABLE
C    12.   SUBROTATION INFORMATION CARDS  FORMAT(2I10)  NO.=NPSI
C          COL. 1-10      IPSVEC(1,J)    FIRST DEFINING ATOM
C          COL.11-20      IPSVEC(2,J)    SECOND DEFINING ATOM
C    13.   POTENTIAL PARAMETER REFERENCE TABLE  FORMAT(36I2)
C          COL. 1- 2      IPRET(1,1)
C          COL. 3- 4      IPRET(1,2)
C          ...
C          COL. VARIES    IPRET(NPRET,NPRET)
C    14.   CELL TRANSLATION CARD  FORMAT(6I5,2F10.2)
C          COL. 1- 5      ITCEL(1)  MAXIMUM NEGATIVE A TRANSLATION
C          COL. 6-10      ITCEL(2)  MAXIMUM NEGATIVE B TRANSLATION
C          ...
C          COL.26-30      ITCEL(6)  MAXIMUM POSITIVE C TRANSLATION
C          COL.31-40      RMAX      MAXIMUM DOJK IN POTENTIAL PARAMETERS
C          COL.41-50      DMAX TO BE ADDED TO DOJK TO DETERMINE SUMMATION
C                           LIMIT
C    15.   PARAMETER CONTROL CARDS FORMAT(72I1)
C          COL. 1         ISEL(1)  +1 IF TO BE VARIED, OR BLANK
C          ...
C          COL.72         ISEL(72)
C          COL. 1         ISEL(73)
C          ...
C          COL.18         ISEL(90)
     16.   ANY CARDS READ BY SUBROUTINE OUTPT
C
C    17.   STOPPER CARD (OR TAPE ASSIGNMENT CARD FOR NEXT PROBLEM)
C                          FORMAT(7(8X,I2))
C          COL. 1-10      NINP
C          COL.11-20      NOUT
C          COL.21-30      KEY       +1 FOR STOPPER
C
C      PARAMETERS ARE ORDERED AS FOLLOWS
C
C           I          PAR(I)
C
C         1- 3         THETA ROTATIONS 1
C         4- 6         TRANSLATIONS 1
C         7- 9         THETA ROTATIONS 2
C        10-12         TRANSLATIONS 2
C        13-24         PSI ROTATIONS
C        25-30         LATTICE CONSTANTS
C        31-34         POTENTIAL PARAMETERS 1
C        35-38         POTENTIAL PARAMETERS 2
C        ...
C        67-70         POTENTIAL PARAMETERS 10
C        71-74         POTENTIAL PARAMETERS 11
C        ...
C        87-90         POTENTIAL PARAMETERS 15
C
C      GLOSSARY OF SYMBOLS
C
C      A1(I,J)-A3(I,J) MATRIX WORK CELLS
C      APSI            SUBROTATION ANGLE
C      C1-C3           CONSTANT WORK CELLS
C      DELTE           ESTIMATE OF E(MODEL)-E(FINAL)
C      DER(I)          DERIVATIVES WITH RESPECT TO THE ITH PARAMETER
C      DINV(I,J)       TRANSFORMS CARTESIAN TO CELL COORDINATES
C      DIST            A DISTANCE
C      DMAT(I,J)       TRANSFORMS CELL TO CARTESIAN COORDINATES
C      DMAX            TO BE ADDED TO DOJK TO DETERMINE SUMMATION LIMIT
C      DSTE(I,J)       EOJK AND DOJK FOR THE JTH ATOM PAIR
```

```
C     EZERO          VALUE OF E FOR CURRENT MODEL
C     E              AN ENERGY
C     GRAD2          GRADIENT SQUARED
C     I              INDEX
C     IA             INDEX FOR ATOM 1
C     IARB           INDEX FOR RB 1
C     IB             INDEX FOR ATOM 2
C     IC             CYCLE NUMBER
C     INCEL          CELL TO CARTESIAN TRANSFORMATION INDICATOR
C     IPOTR(I)       REFERENCE TO IPRET TABLE FOR ITH ATOM
C     IPRET(I,J)     POTENTIAL PARAMETER NO. FOR TYPE IJ INTERACTION
C     IPSI(I)        SUBROTATION GROUP NUMBER FOR ITH ATOM-IF NONE, ZERO
C     IPSVEC(I,J)    TWO ATOM NUMBERS DEFINING THE JTH SUBROTATION
C     IS             SYMMETRY INDEX
C     ISEL(I)        PARAMETER SELECTION INFORMATION
C     ISWIT          SWITCH CONSTANT FOR GNSYM JTWE ROUTINE
C     ITABW          INDEX FOR JKTAB
C     ITCEL(I)       MIN. AND MAX. CELL TRANSLATIONS TO BE CONSIDERED
C     ITHE(I)        RIGID BODY GROUP NUMBER FOR ITH ATOM
C     ITW(I)         WORKING CELL TRANSLATION
C     IX             INDEX
C     J              INDEX
C     JKTAB(I,J)     IA, IB, LTS, AND LSS FOR THE JTH ATOM PAIR
C     JTWE(LTS)      VALUE OF LSS CORRESPONDING TO STWE(I,LTS)
C     K              INDEX
C     KEY            EXIT CODE
C     KSTOP          SWITCH CONSTANT FOR SHIFT AND DELTE ROUTINE
C     L              INDEX
C     LSS            SYMMETRY MATRIX NUMBER
C     LTS            TRANSLATIONAL SYMMETRY NUMBER
C     LTSM           NUMBER OF TRANSLATIONAL SYMMETRIES CONSIDERED
C     M              INDEX
C     N              INDEX
C     NA             NUMBER OF ATOMS IN RIGID BODY
C     NC             NUMBER OF CYCLES
C     NG             ERROR INDICATOR
C     NINP           INPUT TAPE NUMBER
C     NOUT           OUTPUT TAPE NUMBER
C     NPMAX          MAXIMUM NUMBER OF PARAMETERS
C     NPOT           NUMBER OF SETS OF POTENTIAL PARAMETERS
C     NPRET          WORKING DIMENSION OF IPRET TABLE
C     NPSI           NUMBER OF SUBROTATIONS
C     NS             NUMBER OF SYMMETRY CARDS
C     NTHE           NUMBER OF RIGID BODY GROUPS
C     PAR(I)         REFERENCE PARAMETER LIST
C     PARW(I)        WORKING PARAMETER LIST
C     PINC(I)        PARAMETER INCREMENTS
C     PSINC(I,J)     SUBROTATION INCREMENT MATRIX
C     RMAX           LARGEST DOJK IN POTENTIAL PARAMETER LIST
C     RMINC(I,J,K)   ORTHONORMALIZED ROTATION INCREMENT MATRIX FOR RB K
C     RMINP(I,J,K)   INITIAL ROTATION MATRIX FOR RIGID BODY K
C     RTPSI(I,J,K)   SUBROTATION MATRIX K
C     SHIFT          SHIFT FACTOR
C     SS(I,J,K)      SYMMETRY TRANSFORMATION MATRIX FOR KTH OPERATION
C     ST(I,J)        TRANSLATIONAL SYMMETRY VECTOR FOR JTH OPERATION
C     STWE(I,LTS)    TRANSLATIONAL SYMMETRY INCLUDING CELL TRANSLATIONS
C     TITLE(I)       TITLE
C     V1(I)-V5(I)    VECTOR WORK CELLS
C     XC(I,J)        COORDINATES OF JTH ATOM
C     XMAX(I)        MAXIMUM PARAMETERS CONSIDERED BY GNSYM
C     XMIN(I)        MINIMUM PARAMETERS CONSIDERED BY GNSYM
C     XTRAN(I)       INITIAL TRANSLATION
```

```
C      XV(I)          UNIT X VECTOR USED IN RIPSI
C      XZPSI(I,J)     CENTER OF JTH SUBROTATION
C      XZTHE(I,K)     CENTER OF ROTATION OF RIGID BODY K
C      YV(I)          UNIT Y VECTOR USED IN RIPSI
C
       DIMENSION TITLE(15), PAR(90), RMINP(3,3,2), XZTHE(3,2), ST(3,24),
      1  SS(3,3,24), XC(3,100), IPSI(100), IPOTR(100), IPSVEC(2,12),
      2  PARW(90),  IPRET(8,8), ITCEL(6), DMAT(3,3), DINV(3,3), V1(3),
      3  V2(3), V3(3), V4(3), V5(3), A1(3,3),A2(3,3),A3(3,3), XTRAN(3,2),
      4  XMIN(3), XMAX(3), ITW(3), STWE(3,200), JTWE(200),   ISEL(90),
      5  XZPSI(3,12), XV(3), YV(3), PSINC(3,3), RTPSI(3,3,12), ITHE(100),
      6  JKTAB(4,1800), DSTE(2,1800), DER(90), PINC(90), RMINC(3,3,2)
       COMMON NINP, NOUT, TITLE, PAR,  RMINP, XZTHE, NS, NA, NPSI, INCEL,
      1  NPOT, NPRET, DELTE, ST, SS, XC, IPSI, IPOTR, IPSVEC, PARW,IPRET,
      2  ITCEL, RMAX, DMAX, DMAT, DINV, V1, V2, V3, V4, V5, A1, A2, A3,
      3  XTRAN, XMIN, XMAX, I, J, K, L, M, N, IS, IX, IA, IB, LTS,
      4  ITW, ISWIT, STWE, JTWE, LTSM, ITABW, LSS, C1, C2, C3, DIST,
      5  EZERO, ISEL, NC, XZPSI, XV, YV, PSINC, RTPSI, ITHE, JKTAB, DSTE,
      6  DER, PINC, GRAD2, SHIFT, KSTOP, NG, NTHE, E, RMINC, NPMAX
C
       XV(1)=1.0
       XV(2)=0.0
       XV(3)=0.0
       YV(1)=0.0
       YV(2)=1.0
       YV(3)=0.0
  697  READ 7, NINP, NOUT, KEY
    7  FORMAT(7(8X,I2))
       IF (KEY)  698,698,699
  698  CALL INPUT
       CALL ORMAT(PAR(25),DMAT)
       CALL GINV3(DMAT,DINV,NG)
C      TRANSFORM INPUT TO CARTESIAN COORDINATES IF REQUIRED
       IF (INCEL) 1,1,2
    2  DO 3  I=1, NA
       CALL MV(DMAT,XC(1,I),V1)
       DO 3  J=1, 3
    3  XC(J,I)=V1(J)
    1  CONTINUE
C      INITIAL ROTATION AND TRANSLATION
       DO 4  I=1, NA
       IARB=ITHE(I)
       CALL VS(XC(1,I),XZTHE(1,IARB),V1)
       CALL MV(RMINP(1,1,IARB),V1,V2)
       CALL VA(V2,XZTHE(1,IARB),V1)
    4  CALL VA(V1,XTRAN(1,IARB),XC(1,I))
       DO 6 IARB=1, NTHE
       CALL VA(XZTHE(1,IARB),XTRAN(1,IARB),V1)
       DO 6  I=1, 3
    6  XZTHE(I,IARB)=V1(I)
C      SELECT INTERATOMIC VECTORS FOR CONSIDERATION
       CALL GNSYM
C      SET UP INCREMENTS
C      ROTATION IN THETA
       DO 51 I=1, 3
       PINC(I+6)=0.002
   51  PINC(I)=0.002
C      TRANSLATION
       DO 52 I=4, 6
       PINC(I+6)=0.003
   52  PINC(I)=0.003
C      ROTATION IN PSI
```

```
      DO 53 I=13, 24
   53 PINC(I)=0.002
C     LATTICE CONSTANTS
      DO 54 I=25, 27
   54 PINC(I)=0.01
      DO 55 I=28, 30
   55 PINC(I)=0.008
      DO 56 I=31, NPMAX, 4
C     EJKZERO
      PINC(I)=0.001
C     DJKZERO
      PINC(I+1)=0.005
C     RHOJK
      PINC(I+2)=0.004
C     MJK
   56 PINC(I+3)=0.05
C     PREPARE TO BEGIN NO REFINEMENT CYCLES WITH CURRENT JKTAB AND DSTE
C     SET UP INITIAL PARAMETER LIST WITH ZEROS
      DO 11  I=1, 24
   11 PAR(I)=0.0
      IC=0
      IF (NO)  401, 401, 999
  999 IC=IC+1
C     INITIALIZE SUBROTATION MATRICES
      APSI=0.002
      IF (NPSI) 43,43,44
   44 DO 45  J=1, NPSI
   45 CALL RIPSI(J,APSI)
   43 CONTINUE
C     CALCULATE SUMS OF DERIVATIVES
      DO 121 J=1, NPMAX
  121 DER(J)=0.0
      DO 222 J=1, NPMAX
      IF(ISEL(J)) 222,222,123
  123 DO 151 L=1, NPMAX
  151 PARW(L)=PAR(L)
      PARW(J)=PAR(J)+PINC(J)
      CALL PATCH(PARW)
      IF (J-4) 131,125,125
  125 IF (J-7) 132,226,226
  226 IF (J-10) 131,227,227
  227 IF (J-13)  132,126,126
  126 IF (J-25) 133,127,127
  127 IF (J-31) 134,135,135
C     ROTATION PARAMETER
  131 CALL DJKL1(ITABW,JKTAB,XO,PARW,SS,STWE,XZTHE,ITHE,IPRET,IPOTR,E)
      GO TO 122
C     TRANSLATION PARAMETER
  132 CALL DJKL2(ITABW,JKTAB,XO,PARW,SS,STWE,ITHE,IPRET,IPOTR,E)
      GO TO 122
C     SUBROTATION PARAMETER
  133 CALL DJKL3(ITABW,JKTAB,XO,PARW,SS,STWE,IPSI,RTPSI,XZPSI,IPRET,
     1  IPOTR,J,E)
      GO TO 122
C     LATTICE PARAMETER
  134 CALL DJKL4(ITABW,JKTAB,XO,PARW,SS,STWE,OINV,IPRET,IPOTR,E)
      GO TO 122
C     POTENTIAL PARAMETER
  135 E=0.0
      DO 145 I=1, ITABW
      CALL EJKL(I,DSTE(2,I),PARW,JKTAB,IPRET,IPOTR,O1)
  145 E=E+O1
```

```
  122 DER(J)=(E-EZERO)/PINC(J)
  222 CONTINUE
C     CALCULATE GRADIENT SQUARED
      GRAD2=0.0
      DO 161 I=1, NPMAX
      IF (ISEL(I)) 161,161,162
  162 GRAD2=GRAD2+DER(I)*DER(I)
  161 CONTINUE
      SHIFT=DELTE/GRAD2
      DO 165  I=1, NPMAX
      IF (ISEL(I)) 163,163,164
  164 PARW(I)=PAR(I)-SHIFT*DER(I)
      GO TO 165
  163 PARW(I)=PAR(I)
  165 CONTINUE
      CALL PATCH(PARW)
C     ADJUST XC ARRAY FOR NEXT CYCLE
      KSTOP=1
C     OBTAIN ORTHONORMALIZED ROTATION MATRICES
  399 DO 301 IARB=1, NTHE
      K=IARB*6-5
      CALL ROTOR(PARW(K),RMINC(1,1,IARB))
      CALL MM(RMINC(1,1,IARB),RMINP(1,1,IARB),A2)
      DO 301 I=1, 3
      DO 301 J=1, 3
  301 RMINP(I,J,IARB)=A2(I,J)
      DO 302 I=1, NA
      IARB=ITHE(I)
      CALL MV(RMINC(1,1,IARB),XC(1,I),V1)
      DO 302 J=1, 3
      K=6*IARB-3+J
  302 XC(J,I)=V1(J)+PARW(K)
      DO 379  IARB=1, NTHE
      DO 379  J=1, 3
      K=6*IARB-3+J
  379 XZTHE(J,IARB)=XZTHE(J,IARB)+PARW(K)
C     ADJUST FOR SUBROTATIONS
      IF (NPSI) 303,303,304
  304 DO 305  J=1, NPSI
      CALL RIPSI(J,PARW(J+12))
      DO 305  I=1, NA
      IF (J-IPSI(I)) 305,306,305
  306 CALL VS(XC(1,I),XZPSI(1,J),V1)
      CALL MV(RTPSI(1,1,J),V1,V2)
      CALL VA(V2,XZPSI(1,J),XC(1,I))
  305 CONTINUE
C     ADJUST FOR LATTICE CONSTANTS
  303 CALL ORMAT(PARW(25),DMAT)
      CALL MM(DMAT,DINV,A2)
      DO 311 I=1, NA
      CALL MV(A2,XC(1,I),V1)
      DO 311 J=1, 3
  311 XC(J,I)=V1(J)
C     ADJUST STWE AND SS FOR NEW LATTICE CONSTANTS
      DO 501  I=1, LTSM
      CALL MV(A2,STWE(1,I),V1)
      DO 501  J=1, 3
  501 STWE(J,I)=V1(J)
      CALL GINV3(A2,A1,NC)
      DO 502  I=1, NS
      CALL MM(A2,SS(1,1,I),A3)
  502 CALL MM(A3,A1,SS(1,1,I))
```

```
      CALL GINV3(DMAT,DINV,NG)
C     SET UP NEW DSTE TABLE AND CALCULATE NEW EZERO (C1)
      C1=0.0
      DO 312 I=1, ITABW
      IA=JKTAB(1,I)
      IB=JKTAB(2,I)
      LTS=JKTAB(3,I)
      LSS=JKTAB(4,I)
      CALL MV(SS(1,1,LSS),XC(1,IB),V1)
      CALL VA(STWE(1,LTS),V1,V2)
      CALL MAG(V2,XC(1,IA),DSTE(2,I))
      CALL EJKL(I,DSTE(2,I),PARW,JKTAB,IPRET,IPOTR,DSTE(1,I))
      C1=C1+DSTE(1,I)
  312 CONTINUE
C     CHECK NEW VALUE OF EZERO
      IF (EZERO-C1)  313,313,314
  313 DO 315  I=1, 24
      IF (ISEL(I)) 315,315,316
  316 PARW(I)=SHIFT*DER(I)*(2.0**(-KSTOP))
  315 CONTINUE
      DO 371  I=25, NPMAX
      IF (ISEL(I))  371, 371, 372
  372 PARW(I)=PARW(I)+SHIFT*DER(I)*(2.0**(-KSTOP))
  371 CONTINUE
      CALL PATCH(PARW)
      DELTE=DELTE*0.5
      KSTOP=KSTOP+1
      IF (KSTOP-4)  399, 314, 314
C     END OF CYCLE
  314 EZERO=C1
  322 FORMAT(1HO  8H  CYCLE I2,  8H  EZERO=F10.2,    8H  DELTE=F10.4,
     1  8H  GRAD2=F10.2/1HO20H PARAMETER     SHIFT)
  323 FORMAT(1HOI6,F14.5)
      WRITE OUTPUT TAPE NOUT, 322, IC, EZERO, DELTE, GRAD2
      DO 324  I=1, NPMAX
      IF (ISEL(I)) 324,324,325
  325 C2=-SHIFT*DER(I)*(2.0**(1-KSTOP))
      WRITE OUTPUT TAPE NOUT, 323, I, C2
  324 CONTINUE
      DO 321  I=25, NPMAX
  321 PAR(I)=PARW(I)
      IF (IC-NC) 999,401,401
  401 CALL OUTPT
      GO TO 697
  699 STOP 87
      END


     END       ACCNTA0015  @D.WILLIAMS@                                    PCGC
     START     ACCNTA0015  @D.WILLIAMS@                                    PCGC
     COMPILE   RUN  FORTRAN LIST                                           PCGC
C     SUBROUTINE GNSYM
      SUBROUTINE GNSYM
      DIMENSION TITLE(15), PAR(90), RMINP(3,3,2), XZTHE(3,2), ST(3,24),
     1  SS(3,3,24), XC(3,100), IPSI(100), IPOTR(100), IPSVEC(2,12),
     2  PARW(90),  IPRET(8,8), ITCEL(6), DMAT(3,3), DINV(3,3), V1(3),
     3  V2(3), V3(3), V4(3), V5(3), A1(3,3),A2(3,3),A3(3,3), XTRAN(3,2),
     4  XMIN(3), XMAX(3), ITW(3), STWE(3,200), JTWE(200),   ISEL(90),
     5  XZPSI(3,12), XV(3), YV(3), PSINC(3,3), RTPSI(3,3,12), ITHE(100),
     6  JKTAB(4,1800), DSTE(2,1800), DER(90), PINC(90), RMINC(3,3,2)
      COMMON NINP, NOUT, TITLE, PAR,  RMINP, XZTHE, NS, NA, NPSI, INCEL,
     1  NPOT, NPRET, DELTE, ST, SS, XC, IPSI, IPOTR, IPSVEC, PARW,IPRET,
```

```
     2  ITCEL, RMAX, DMAX, DMAT, DINV, V1, V2, V3, V4, V5, A1, A2, A3,
     3  XTRAN, XMIN, XMAX, I, J, K, L, M, N, IS, IX, IA, IB, LTS,
     4  ITW, ISWIT, STWE, JTWE, LTSM, ITABW, LSS, C1, C2, C3, DIST,
     5  EZERO, ISEL, NC, XZPSI, XV, YV, PSINC, RTPSI, ITHE, JKTAB, DSTE,
     6  DER, PINC, GRAD2, SHIFT, KSTOP, NG, NTHE, E, RMINC, NPMAX
      DIMENSION TCELL(3), TSYM(3)
C     ORTHOGONALIZE SYMMETRY MATRICES
      DO 101 I=1, NS
      CALL MV(DMAT,ST(1,I),V1)
      DO 123  J=1, 3
  123 ST(J,I)=V1(J)
      CALL MM(SS(1,1,I),DINV,A1)
  101 CALL MM(DMAT,A1,SS(1,1,I))
C     FIND MAX AND MIN XC VALUES
      C1=0.5*(RMAX+DMAX)
      DO 20 IX=1, 3
      XMIN(IX)=100000.0
      XMAX(IX)=-100000.0
      DO 1  IA=1, NA
      IF (XC(IX,IA)-XMIN(IX)) 4,5,5
    4 XMIN(IX)=XC(IX,IA)
    5 IF (XC(IX,IA)-XMAX(IX)) 1,1,6
    6 XMAX(IX)=XC(IX,IA)
    1 CONTINUE
      XMAX(IX)=XMAX(IX)+C1
      XMIN(IX)=XMIN(IX)-C1
   20 CONTINUE
C     SELECT APPLICABLE CELL TRANSLATIONS
C     FIRST SYMMETRY CARD IS  X Y Z , I.E., ASYMMETRIC UNIT
C     INTRAMOLECULAR DISTANCES AND INTER RIGID BODY DISTANCES
      JTWE(1)=1
      DO 79 J=1, 3
   79 STWE(J,1)=ST(J,1)
      LTS=1
      DO 41 I=1, 3
   41 ITW(I)=ITCEL(I)
   61 DO 75 I=1, 3
   75 V2(I)=FLOATF(ITW(I))
      CALL MV(DMAT,V2,TCELL)
      DO 62 IS=1, NS
C     REJECT INTRAMOLECULAR DISTANCES IN THIS SECTION
      IF (IS+XABSF(ITW(1))+XABSF(ITW(2))+XABSF(ITW(3))-1) 62,62,43
   43 CALL VA(TCELL,ST(1,IS),TSYM)
      CALL MV(SS(1,1,IS),XMAX,V4)
      CALL MV(SS(1,1,IS),XMIN,V5)
      CALL VA(TSYM,V4,V1)
      CALL VA(TSYM,V5,V2)
      DO 51  IX=1, 3
      IF (XMAX(IX)-V1(IX)) 53, 52, 52
   52 IF (V1(IX)-XMIN(IX)) 53, 51, 51
   53 IF (XMAX(IX)-V2(IX)) 62, 54, 54
   54 IF (V2(IX)-XMIN(IX)) 62, 51, 51
   51 CONTINUE
C     INCLUDE TRANSLATION-SYMMETRY COMBINATION IN JTWE TABLE
      LTS=LTS+1
      DO 57 I=1, 3
   57 STWE(I,LTS)=TSYM(I)
      JTWE(LTS)=IS
   62 CONTINUE
      DO 60 I=1, 3
      IF (ITW(I)-ITCEL(I+3)) 59,60,60
   59 ITW(I)=ITW(I)+1
```

```
      GO TO 61
   60 ITW(I)=ITCEL(I)
      LTSM=LTS
C     SELECT INDIVIDUAL INTERATOMIC VECTORS FOR JKTAB(JATOM,KATOM,
C       LTS,LSS,ITABW)   DIMENSION(4,1500) OR SO
C     SET UP DSTE TABLE AND CALCULATE EZERO
      EZERO=0.0
      ITABW=0
      DO 71  LTS=1, LTSM
      LSS=JTWE(LTS)
      DO 71 IB=1, NA
      CALL MV(SS(1,1,LSS),XC(1,IB),V1)
      CALL VA(STWE(1,LTS),V1,V2)
      K=IPOTR(IB)
      DO 71 IA=1, NA
C     CHECK ITHE AND IPSI EQUALITY WHEN LTS=1
      IF (LTS-1)  91, 92, 91
   92 IF (ITHE(IA)-ITHE(IB)) 91, 93, 91
   93 IF (IPSI(IA)-IPSI(IB)) 94, 71, 94
   94 IF (IPSI(IA))  71, 71, 95
   95 IF (IPSI(IB))  71, 71, 91
   91 CALL VS(V2,XC(1,IA),V1)
      DIST=SQRTF(V1(1)*V1(1)+V1(2)*V1(2)+V1(3)*V1(3))
      J=IPOTR(IA)
      L=IPRET(J,K)
      C1=PAR(4*L+28)
      IF (DIST-DMAX-C1)  80,80,71
   80 ITABW=ITABW+1
      JKTAB(1,ITABW)=IA
      JKTAB(2,ITABW)=IB
      JKTAB(3,ITABW)=LTS
      JKTAB(4,ITABW)=LSS
      DSTE(2,ITABW)=DIST
      CALL EJKL(ITABW,DIST,PAR, JKTAB,IPRET,IPOTR,DSTE(1,ITABW))
      EZERO=EZERO+DSTE(1,ITABW)
   71 CONTINUE
C     OUTPUT GENSYM INFORMATION
      WRITE OUTPUT TAPE NOUT, 85, NS, LTSM,      ITABW, EZERO,
     1  (XMIN(I), XMAX(I), I=1, 3)
   85 FORMAT (1HO 5H  NS=I2,7H  LTSM=I2,           8H  ITABW=I4,
     1  8H  EZERO=F8.4,
     2  /1HO       8H  XMIN1=F7.2,      8H  XMAX1=F7.2,
     3             8H  XMIN2=F7.2,      8H  XMAX2=F7.2,
     4             8H  XMIN3=F7.2,      8H  XMAX3=F7.2)
      RETURN
      END


      END        ACCNTA0015  @D.WILLIAMS@                                    PCGO
      START      ACCNTA0015  @D.WILLIAMS@                                    PCGO
      COMPILE    RUN  FORTRAN LIST                                           PCGO
C     SUBROUTINE INPUT
      SUBROUTINE INPUT
      DIMENSION TITLE(15), PAR(90), RMINP(3,3,2), XZTHE(3,2), ST(3,24),
     1  SS(3,3,24), XC(3,100), IPSI(100), IPOTR(100), IPSVEC(2,12),
     2  PARW(90),  IPRET(8,8), ITCEL(6), DMAT(3,3), DINV(3,3), V1(3),
     3  V2(3), V3(3), V4(3), V5(3), A1(3,3),A2(3,3),A3(3,3), XTRAN(3,2),
     4  XMIN(3), XMAX(3), ITW(3), STWE(3,200), JTWE(200),   ISEL(90),
     5  XZPSI(3,12), XV(3), YV(3), PSINC(3,3), RTPSI(3,3,12), ITHE(100),
     6  JKTAB(4,1800), DSTE(2,1800), DER(90), PINC(90), RMINC(3,3,2)
      COMMON NINP, NOUT, TITLE, PAR,  RMINP, XZTHE, NS, NA, NPSI, INCEL,
     1  NPOT, NPRET, DELTE, ST, SS, XC, IPSI, IPOTR, IPSVEC, PARW,IPRET,
```

```
     2  ITCEL, RMAX, DMAX, DMAT, DINV, V1, V2, V3, V4, V5, A1, A2, A3,
     3  XTRAN, XMIN, XMAX, I, J, K, L, M, N, IS, IX, IA, IB, LTS,
     4  ITH, ISWIT, STHE, JTHE, LTSM, ITABH, LSS, C1, C2, C3, DIST,
     5  EZERO, ISEL, NC, XZPSI, XV, YV, PSINC, RTPSI, ITHE, JKTAB, DSTE,
     6  DER, PINC, GRAD2, SHIFT, KSTOP, NG, NTHE, E, RMINC, NPMAX
    2 FORMAT(14A5,A2)
      READ INPUT TAPE NINP, 2, (TITLE(I),I=1,15)
    3 FORMAT(1HO14A5,A2)
      WRITE OUTPUT TAPE NOUT, 3, (TITLE(I),I=1,15)
   41 FORMAT(8I5,F10.4)
      READ INPUT TAPE NINP, 41, NS, NA, NTHE, NPSI, NPOT, NPRET, INCEL,
     1  NC, DELTE
   10 FORMAT(1HO  5H  NS=I2,5H  NA=I2,7H  NTHE=I2,  7H  NPSI=I2,
     1  7H  NPOT=I2,  8H  NPRET=I2,  8H  INCEL=I2,  5H  NC=I2,
     2  8H  DELTE=F10.5)
      WRITE OUTPUT TAPE NOUT, 10, NS, NA, NTHE, NPSI, NPOT, NPRET,
     1  INCEL, NC, DELTE
    6 FORMAT(9F8.2)
    8 FORMAT(6F10.2)
      DO 51 K=1, NTHE
      READ INPUT TAPE NINP, 6, ((RMINP(I,J,K),J=1,3),I=1,3)
      READ INPUT TAPE NINP, 8, (XZTHE(I,K),I=1,3), (XTRAN(I,K),I=1,3)
    7 FORMAT(1HO  7H  RMINPI1,  9F10.6)
    9 FORMAT(1HO  7H  XZTHEI1, 3F10.2,7H  XTRANI1, 3F10.2)
      WRITE OUTPUT TAPE NOUT, 7, K, ((RMINP(I,J,K),J=1,3),I=1,3)
   51 WRITE OUTPUT TAPE NOUT, 9, K, (XZTHE(I,K),I=1,3),K,(XTRAN(I,K),
     1  I=1,3)
    4 FORMAT(6F10.4)
      READ INPUT TAPE NINP, 4,  (PAR(I), I=25, 30)
    5 FORMAT(1HO 20H  LATTICE CONSTANTS 3F10.4,3F10.2)
      WRITE OUTPUT TAPE NOUT, 5, (PAR(I), I=25,30)
      DO 29  I=28, 30
   29 PAR(I)=PAR(I)/57.29578
   17 FORMAT(4F10.5,32X)
      NPMAX=4*NPOT+30
      READ INPUT TAPE NINP, 17,  (PAR(J), J=31,NPMAX)
   18 FORMAT(1HO 24H  POTENTIAL PARAMETERS  /1H (/1H 4F10.5))
      WRITE OUTPUT TAPE NOUT, 18, (PAR(J), J=31,NPMAX)
   11 FORMAT(3F10.8,9F4.0,6X)
      READ INPUT TAPE NINP, 11, ((ST(I,K),I=1,3),((SS(N,J,K),J=1,3),
     1  N=1,3),K=1,NS)
   12 FORMAT(1HO 22H  SYMMETRY INFORMATION/1H /(1H 3F12.8,9F8.1))
      WRITE OUTPUT TAPE NOUT, 12, ((ST(I,K),I=1,3),((SS(N,J,K),J=1,3),
     1  N=1,3),K=1,NS)
   13 FORMAT(3F10.8,3I10,12X)
      READ INPUT TAPE NINP, 13, ((XC(I,K),I=1,3),ITHE(K),IPSI(K),
     1  IPCTR(K),K=1,NA)
   14 FORMAT(1HO 20H  ATOMIC INFORMATION16X,7HITHE(I)3X,7HIPSI(I)3X,
     1  8HIPOTR(I)      /(1H 3F10.6,4I10))
      WRITE OUTPUT TAPE NOUT, 14, ((XC(I,K),I=1,3),ITHE(K),IPSI(K),
     1  IPCTR(K),K,K=1,NA)
   15 FORMAT(2I10)
      IF (NPSI) 42, 42, 43
   43 READ INPUT TAPE NINP, 15, ((IPSVEC(I,J),I=1,2),J=1,NPSI)
   16 FORMAT(1HO 50H  SUBROTATION INFORMATION        IPSVEC(1,J)
     1 30H        IPSVEC(2,J)           J
     2  /1H /(1H 26X,I10,I25,I17))
      WRITE OUTPUT TAPE NOUT, 16, ((IPSVEC(I,J),I=1,2),J,J=1,NPSI)
   19 FORMAT(36I2)
   42 READ INPUT TAPE NINP, 19, ((IPRET(I,J),J=1,NPRET),I=1,NPRET)
   20 FORMAT(1HO 10H  IPRET   36I2)
      WRITE OUTPUT TAPE NOUT,20,((IPRET(I,J),J=1,NPRET),I=1,NPRET)
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```
   21 FORMAT(6I5,2F10.2)
      READ INPUT TAPE NINP, 21, (ITCEL(I),I=1,6), RMAX, DMAX
   22 FORMAT(1HC 10H  ITCEL   6I5,    7H  RMAX=F 6.2,7H  DMAX=F 6.2)
      WRITE OUTPUT TAPE NOUT, 22, (ITCEL(I),I=1,6), RMAX, DMAX
      READ INPUT TAPE NINP, 31,(ISEL(I), I=1,NPMAX)
   31 FORMAT(72I1)
      WRITE OUTPUT TAPE NOUT, 32, (ISEL(I),I=1,NPMAX)
   32 FORMAT(1HO 25H  PARAMETERS SELECTED          /1HO2X,
     1      4(3I1,1X),12I1,1X,6I1,2X,15(4I1,1X))
      RETURN
      END

      END        ACCNTA0015  @D.WILLIAMS@                                    PCGO
      START      ACCNTA0015  @D.WILLIAMS@                                    PCGO
      COMPILE    RUN  FORTRAN LIST                                           PCGO
C      SUBROUTINE RIPSI(JJ,APSI)
       SUBROUTINE RIPSI(JJ,APSI)
       DIMENSION TITLE(15), PAR(90), RMINP(3,3,2), XZTHE(3,2), ST(3,24),
      1  SS(3,3,24), XC(3,100), IPSI(100), IPOTR(100), IPSVEC(2,12),
      2  PARW(90),  IPRET(8,8), ITCEL(6), DMAT(3,3), DINV(3,3), V1(3),
      3  V2(3), V3(3), V4(3), V5(3), A1(3,3),A2(3,3),A3(3,3), XTRAN(3,2),
      4  XMIN(3), XMAX(3), ITW(3), STWE(3,200), JTWE(200),   ISEL(90),
      5  XZPSI(3,12), XV(3), YV(3), PSINC(3,3), RTPSI(3,3,12), ITHE(100),
      6  JKTAB(4,1800), DSTE(2,1800), DER(90), PINC(90), RMINC(3,3,2)
       COMMON NINP, NOUT, TITLE, PAR,  RMINP, XZTHE, NS, NA, NPSI, INCEL,
      1  NPOT, NPRET, DELTE, ST, SS, XC, IPSI, IPOTR, IPSVEC, PARW,IPRET,
      2  ITCEL, RMAX, DMAX, DMAT, DINV, V1, V2, V3, V4, V5, A1, A2, A3,
      3  XTRAN, XMIN, XMAX, I, J, K, L, M, N, IS, IX, IA, IB, LTS,
      4  ITW, ISWIT, STWE, JTWE, LTSM, ITABW, LSS, C1, C2, C3, DIST,
      5  EZERO, ISEL, NC, XZPSI, XV, YV, PSINC, RTPSI, ITHE, JKTAB, DSTE,
      6  DER, PINC, GRAD2, SHIFT, KSTOP, NG, NTHE, E, RMINC, NPMAX
       PSINC(1,1)=1.0
       PSINC(1,2)=0.0
       PSINC(1,3)=0.0
       PSINC(2,1)=0.0
       PSINC(2,2)=COSF(APSI)
       PSINC(2,3)=SINF(APSI)
       PSINC(3,1)=0.0
       PSINC(3,2)=-PSINC(2,3)
       PSINC(3,3)=PSINC(2,2)
       I=IPSVEC(1,JJ)
       DO 2  K=1, 3
    2  XZPSI(K,JJ)=XC(K,I)
       K=IPSVEC(2,JJ)
       CALL VS(XC(1,K),XC(1,I),V1)
       CALL NORM(V1,A1(1,1))
       IF (ABSF(V1(2))+ABSF(V1(3))) 3, 3, 4
    3  CALL VXV(V1,YV,V2)
       GO TO 5
    4  CALL VXV(V1,XV,V2)
    5  CALL NORM(V2,A1(1,2))
       CALL VXV(A1(1,1),A1(1,2),A1(1,3))
       CALL GINV3(A1,A2,NG)
       CALL MM(PSINC,A2,A3)
       CALL MM(A1,A3,RTPSI(1,1,JJ))
    9  RETURN
       END

      END        ACCNTA0015  @D.WILLIAMS@                                    PCGO
      START      ACCNTA0015  @D.WILLIAMS@                                    PCGO
```

```
      COMPILE   RUN  FORTRAN LIST                                                PCGC
C      SUBROUTINE DJKL1   ROTATION PARAMETER
       SUBROUTINE DJKL1(ITABW,JKTAB,XC,PARW,SS,STWE,XZTHE,ITHE,IPRET,
      1  IPCTR, E)
       DIMENSION JKTAB(4,1800), XC(3,100), PARW(90), SS(3,3,24),
      1  STWE(3,200),XZTHE(3,2), ITHE(100), IPRET(8,8), IPCTR(100)
       DIMENSION R(3,3,2), V1(3), V2(3), V3(3)
       E=0.0
       R(1,2,1)=-PARW(3)
       R(1,3,1)= PARW(2)
       R(2,3,1)=-PARW(1)
       R(1,2,2)=-PARW(9)
       R(1,3,2)= PARW(8)
       R(2,3,2)=-PARW(7)
       DO 2  J=1, 2
       DO 2  K=1, 3
       DO 1  KK=K, 3
     1 R(KK,K,J)=-R(K,KK,J)
     2 R(K,K,J)=1.0
       DO 3  I=1, ITABW
       IA=JKTAB(1,I)
       IB=JKTAB(2,I)
       LTS=JKTAB(3,I)
       LSS=JKTAB(4,I)
       IARB=ITHE(IA)
       IBRB=ITHE(IB)
       CALL VS(XC(1,IA),XZTHE(1,IARB),V1)
       CALL MV(R(1,1,IARB),V1,V2)
       CALL VA(V2,XZTHE(1,IARB),V1)
       CALL VS(XC(1,IB),XZTHE(1,IBRB),V2)
       CALL MV(R(1,1,IBRB),V2,V3)
       CALL VA(V3,XZTHE(1,IBRB),V2)
       CALL MV(SS(1,1,LSS),V2,V3)
       CALL VA(STWE(1,LTS),V3,V2)
       CALL MAG(V1,V2,DIST)
       CALL EJKL(I,DIST,PARW,JKTAB,IPRET,IPCTR,C1)
       E=E+C1
     3 CONTINUE
       RETURN
       END


      END        ACCNTA0015  @D.WILLIAMS@                                        PCGC
      START      ACCNTA0015  @D.WILLIAMS@                                        PCGC
      COMPILE    RUN  FORTRAN LIST                                               PCGC
C      SUBROUTINE DJKL2   TRANSLATION PARAMETER
       SUBROUTINE DJKL2(ITABW,JKTAB,XC,PARW,SS,STWE,ITHE,IPRET,IPCTR,E)
       DIMENSION JKTAB(4,1800), XC(3,100), PARW(90), SS(3,3,24),
      1  STWE(3,200),ITHE(100), IPRET(8,8), IPCTR(100)
       DIMENSION V1(3),V2(3),V3(3)
       E=0.0
       DO 1 I=1,ITABW
       IA=JKTAB(1,I)
       IB=JKTAB(2,I)
       LTS=JKTAB(3,I)
       LSS=JKTAB(4,I)
       IARB=ITHE(IA)*6-2
       IBRB=ITHE(IB)*6-2
       CALL VA(XC(1,IA),PARW(IARB),V1)
       CALL VA(XC(1,IB),PARW(IBRB),V2)
       CALL MV(SS(1,1,LSS),V2,V3)
       CALL VA(STWE(1,LTS),V3,V2)
```

```
      CALL MAG(V1,V2,DIST)
      CALL EJKL(I,DIST,PARW,JKTAB,IPRET,IPOTR,C1)
      E=E+C1
    1 CONTINUE
      RETURN
      END
```

```
      END        ACCNTA0015  @D.WILLIAMS&                                  PCGO
      START      ACCNTA0015  @D.WILLIAMS&                                  PCGO
      COMPILE    RUN  FORTRAN LIST                                         PCGO
C     SUBROUTINE DJKL3   SUBROTATION PARAMETER
      SUBROUTINE DJKL3(ITABW,JKTAB,XC,PARW,SS,STWE,IPSI,RTPSI,XZPSI,
     1  IPRET,IPOTR,J,E)
      DIMENSION JKTAB(4,1800), XC(3,100), PARW(90), SS(3,3,24),
     1  STWE(3,200),IPSI(100), RTPSI(3,3,12),XZPSI(3,12),IPRET(8,8),
     1  IPOTR(100)
      DIMENSION V1(3),V2(3),V3(3)
      E=0.0
      JPSI=J-12
      DO 10 I=1, ITABW
      IA=JKTAB(1,I)
      IB=JKTAB(2,I)
      LTS=JKTAB(3,I)
      LSS=JKTAB(4,I)
      IAP=IPSI(IA)
      IBP=IPSI(IB)
      IF (IAP-JPSI)  1, 2, 1
    1 DO 3 N=1, 3
    3 V1(N)=XC(N,IA)
      GO TO 4
    2 CALL VS(XC(1,IA),XZPSI(1,IAP),V1)
      CALL MV(RTPSI(1,1,IAP),V1,V2)
      CALL VA(V2,XZPSI(1,IAP),V1)
    4 IF (IBP-JPSI)  5, 6, 5
    5 DO 7 N=1, 3
    7 V2(N)=XC(N,IB)
      GO TO 8
    6 CALL VS(XC(1,IB),XZPSI(1,IBP),V2)
      CALL MV(RTPSI(1,1,IBP),V2,V3)
      CALL VA(V3,XZPSI(1,IBP),V2)
    8 CALL MV(SS(1,1,LSS),V2,V3)
      CALL VA(STWE(1,LTS),V3,V2)
      CALL MAG(V1,V2,DIST)
      CALL EJKL(I,DIST,PARW,JKTAB,IPRET,IPOTR,C1)
      E=E+C1
   10 CONTINUE
      RETURN
      END
```

```
      END        ACCNTACC15  @D.WILLIAMS&                                  PCGC
      START      ACCNTA0015  @D.WILLIAMS&                                  PCGC
      COMPILE    RUN  FORTRAN LIST                                         PCGC
C     SUBROUTINE DJKL4   LATTICE PARAMETER
      SUBROUTINE DJKL4(ITABW,JKTAB,XC,PARW,SS,STWE,DINV,IPRET,IPOTR,E)
      DIMENSION JKTAB(4,1800), XC(3,100), PARW(90), SS(3,3,24),
     1  STWE(3,200),DINV(3,3), IPRET(8,8), IPOTR(100)
      DIMENSION A1(3,3), V1(3), V2(3), V3(3), DINC(3,3)
      E=0.0
      CALL ORMAT(PARW(25),DINC)
      CALL MM(DINC,DINV,A1)
```

```
      DO 1 I=1, ITABM
      IA=JKTAB(1,I)
      IB=JKTAB(2,I)
      LTS=JKTAB(3,I)
      LSS=JKTAB(4,I)
      CALL MV(A1,XC(1,IA),V1)
      CALL MV(SS(1,1,LSS),XC(1,IB),V2)
      CALL VA(STWE(1,LTS),V2,V3)
      CALL MV(A1,V3,V2)
      CALL MAG(V1,V2,DIST)
      CALL EJKL(I,DIST,PARM,JKTAB,IPRET,IPOTR,C1)
      E=E+C1
    1 CONTINUE
      RETURN
      END
```

Page 29, lines 7, 8 and 9 should be:

```
      CALL MV(SS(1, 1, LSS), XC(1, IB), V2)
      CALL VA(STWE(1, LTS), V2, V3)
      CALL MV(A1, V3, V2)
```

```
      END       ACCNTA0015  @D.WILLIAMS@                              PCGO
      START     ACCNTA0015  @D.WILLIAMS@                              PCGO
      COMPILE   RUN  FORTRAN LIST                                     PCGO
C     SUBROUTINE ROTCR(A,B)   OBTAIN ORTHONORMALIZED ROTATION MATRIX
      SUBROUTINE ROTCR(A,B)
      DIMENSION A(3), B(3,3)
      THETA=SQRTF(1.0-0.25*(A(1)*A(1)+A(2)*A(2)+A(3)*A(3)))
      XI=0.5*A(1)
      ETA=0.5*A(2)
      ZETA=0.5*A(3)
      B(1,1)=XI*XI-ETA*ETA-ZETA*ZETA+THETA*THETA
      B(2,1)=2.0*(XI*ETA+ZETA*THETA)
      B(3,1)=2.0*(XI*ZETA-ETA*THETA)
      B(1,2)=2.0*(XI*ETA-ZETA*THETA)
      B(2,2)=-XI*XI+ETA*ETA-ZETA*ZETA+THETA*THETA
      B(3,2)=2.0*(ETA*ZETA+XI*THETA)
      B(1,3)=2.0*(XI*ZETA+ETA*THETA)
      B(2,3)=2.0*(ETA*ZETA-XI*THETA)
      B(3,3)=-XI*XI-ETA*ETA+ZETA*ZETA+THETA*THETA
      RETURN
      END
```

```
      END       ACCNTA0015  @D.WILLIAMS@                              PCGO
      START     ACCNTA0015  @D.WILLIAMS@                              PCGO
      COMPILE   RUN  FORTRAN LIST                                     PCGO
C     INVERT 3X3 MATRIX
      SUBROUTINE GINV3(A,B,NG)
      DIMENSION A(3,3), B(3,3)
      D=A(1,1)*(A(2,2)*A(3,3)-A(2,3)*A(3,2))
     1 -A(1,2)*(A(2,1)*A(3,3)-A(2,3)*A(3,1))
     2 +A(1,3)*(A(2,1)*A(3,2)-A(2,2)*A(3,1))
      IF (ABSF(D)-10.0E-25)  2, 2, 1
    2 NG=1
      GO TO 99
    1 D=1.0/D
      B(1,1)=D*(A(2,2)*A(3,3)-A(2,3)*A(3,2))
      B(2,1)=D*(A(2,3)*A(3,1)-A(2,1)*A(3,3))
      B(3,1)=D*(A(2,1)*A(3,2)-A(2,2)*A(3,1))
      B(1,2)=D*(A(1,3)*A(3,2)-A(1,2)*A(3,3))
      B(2,2)=D*(A(1,1)*A(3,3)-A(1,3)*A(3,1))
      B(3,2)=D*(A(1,2)*A(3,1)-A(1,1)*A(3,2))
      B(1,3)=D*(A(1,2)*A(2,3)-A(1,3)*A(2,2))
      B(2,3)=D*(A(1,3)*A(2,1)-A(1,1)*A(2,3))
      B(3,3)=D*(A(1,1)*A(2,2)-A(1,2)*A(2,1))
```

```
      NG=C
   99 RETURN
      END
```

```
      END       ACCNTA0015  @D.WILLIAMS@                          PCGC
      START     ACCNTA0015  @D.WILLIAMS@                          PCGC
      COMPILE   RUN  FORTRAN LIST                                 PCGC
C      SUBROUTINE ORMAT
       SUBROUTINE ORMAT(ALAT,DMAT)
       DIMENSION ALAT(6), DMAT(3,3)
       SIN6=SINF(ALAT(6))
       COS5=COSF(ALAT(5))
       COS4=COSF(ALAT(4))
       COS6=COSF(ALAT(6))
       VV=1.0-COS4*COS4-COS5*COS5-COS6*COS6+2.0*COS4*COS5*COS6
       VV=SQRTF(VV)
       DMAT(1,1)=ALAT(1)*SIN6
       DMAT(1,2)=0.0
       V=(COS5-COS4*COS6)/SIN6
       DMAT(1,3)=ALAT(3)*V
       DMAT(2,1)=ALAT(1)*COS6
       DMAT(2,2)=ALAT(2)
       DMAT(2,3)=ALAT(3)*COS4
       DMAT(3,1)=0.0
       DMAT(3,2)=0.0
       DMAT(3,3)=ALAT(3)*VV/SIN6
       RETURN
       END
```

```
      END       ACCNTA0015  @D.WILLIAMS@                          PCGD
      START     ACCNTA0015  @D.WILLIAMS@                          PCGD
      COMPILE   RUN  FORTRAN LIST                                 PCGD
C      SUBROUTINE MM(A,B,C)
       SUBROUTINE MM(A,B,C)
       DIMENSION A(3,3), B(3,3), C(3,3)
       DO 1  I=1, 3
       DO 1  J=1, 3
       C(I,J)=0.0
       DO 1  K=1, 3
     1 C(I,J)=C(I,J)+A(I,K)*B(K,J)
       RETURN
       END
```

```
      START     ACCNTA0015  @D.WILLIAMS@                          PCGC
      COMPILE.  RUN  FORTRAN LIST                                 PCGC
C      SUBROUTINE MV(A,B,C)
       SUBROUTINE MV(A,B,C)
       DIMENSION A(3,3), B(3), C(3)
       DO 1  I=1, 3
       C(I)=0.0
       DO 1  J=1, 3
     1 C(I)=C(I)+A(I,J)*B(J)
       RETURN
       END
```

```
      END       ACCNTA0015  @D.WILLIAMS@                          PCGC
      START     ACCNTA0015  @D.WILLIAMS@                          PCGC
      COMPILE   RUN  FORTRAN LIST                                 PCGC
```

```
C      SUBROUTINE VA(A,B,C)
       SUBROUTINE VA(A,B,C)
       DIMENSION A(3), B(3), C(3)
       DO 1  I=1, 3
     1 C(I)=A(I)+B(I)
       RETURN
       END

      END        ACCNTA0C15  @D.WILLIAMS@                              PCGO
      START      ACCNTA0C15  @D.WILLIAMS@                              PCGO
      COMPILE    RUN  FORTRAN LIST                                     PCGO
C      SUBROUTINE VS(A,B,C)
       SUBROUTINE VS(A,B,C)
       DIMENSION A(3), B(3), C(3)
       DO 1  I=1, 3
     1 C(I)=A(I)-B(I)
       RETURN
       END

      END        ACCNTA0C15  @D.WILLIAMS@                              PCGO
      START      ACCNTA0C15  @D.WILLIAMS@                              PCGO
      COMPILE    RUN  FORTRAN LIST                                     PCGO
       SUBROUTINE VXV(A, B, C)
       DIMENSION A(3), B(3), C(3)
       C(1)=A(2)*B(3)-A(3)*B(2)
       C(2)=A(3)*B(1)-A(1)*B(3)
       C(3)=A(1)*B(2)-A(2)*B(1)
       RETURN
       END

      END        ACCNTA0C15  @D.WILLIAMS@                              PCGO
      START      ACCNTA0C15  @D.WILLIAMS@                              PCGO
      COMPILE    RUN  FORTRAN LIST                                     PCGO
C      SUBROUTINE NORM(A,B)
       SUBROUTINE NORM(A,B)
       DIMENSION A(3), B(3)
       C1=SQRTF(A(1)*A(1)+A(2)*A(2)+A(3)*A(3))
       DO 1  I=1, 3
     1 B(I)=A(I)/C1
       RETURN
       END

      END        ACCNTA0C15  @D.WILLIAMS@                              PCGO
      START      ACCNTA0C15  @D.WILLIAMS@                              PCGO
      COMPILE    RUN  FORTRAN LIST                                     PCGO
C      SUBROUTINE MAG(A,B,DIST)
       SUBROUTINE MAG(A,B,DIST)
       DIMENSION A(3), B(3)
       DO 1  I=1, 3
     1 A(I)=A(I)-B(I)
       DIST=SQRTF(A(1)*A(1)+A(2)*A(2)+A(3)*A(3))
       RETURN
       END

      END        ACCNTA0C15  @D.WILLIAMS@                              PCGO
      START      ACCNTA0C15  @D.WILLIAMS@                              PCGO
      COMPILE    RUN  FORTRAN LIST                                     PCGO
```

```
C     SUBROUTINE FJKL(I,DIST,PARW,JKTAB,IPRET,IPCTR,C1)
      SUBROUTINE FJKL(I,DIST,PARW,JKTAB,IPRET,IPCTR,C1)
      DIMENSION PARW(90), JKTAB(4,1800), IPRET(8,8), IPCTR(100)
      IA=JKTAB(1,I)
      IB=JKTAB(2,I)
      J=IPCTR(IA)
      K=IPCTR(IB)
      IP=IPRET(J,K)
      N=27+4*IP
      C1=PARW(N+3)*PARW(N+2)/PARW(N+1)
      C2=(PARW(N+1)-DIST)/PARW(N+2)
      C2=C1*EXPF(C2)
      C3=(PARW(N+1)/DIST)**PARW(N+3)
      C1=PARW(N)*(C3-C2)/(1.0-C1)
      RETURN
      END


     END        ACCNTA0015  @D.WILLIAMS@                                    PCGC
     START      ACCNTA0015  @D.WILLIAMS@                                    PCGC
     COMPILE    RUN  FORTRAN LIST                                           PCGC
C     SUBROUTINE OUTPT
C     INPUT IS ONE CONTROL CARD FORMAT(2F10.2,10I5,I2)
C       COL.  1-10  DLIST - LIST DISTANCES THIS MUCH OR LESS THAN DOJK
C       COL. 11-20  BTEMP - TEMPERATURE FACTOR FOR LSSF CARDS
C       COL. 71-72  ICARD -  =0 FOR NO CARDS OUTPUT
C                            =1 FOR RECYCLE CARDS
C                            =2 FOR BOTH RECYCLE CARDS AND LSSF CARDS
C
      SUBROUTINE OUTPT
      DIMENSION TITLE(15), PAR(90), RMINP(3,3,2), XZTHE(3,2), ST(3,24),
     1  SS(3,3,24), XC(3,100), IPSI(100), IPCTR(100), IPSVEC(2,12),
     2  PARW(90),  IPRET(8,8), ITCEL(6), DMAT(3,3), DINV(3,3), V1(3),
     3  V2(3), V3(3), V4(3), V5(3), A1(3,3),A2(3,3),A3(3,3), XTRAN(3,2),
     4  XMIN(3), XMAX(3), ITW(3), STWE(3,200), JTWE(200),   ISEL(90),
     5  XZPSI(3,12), XV(3), YV(3), PSINC(3,3), RTPSI(3,3,12), ITHE(100),
     6  JKTAB(4,1800), DSTE(2,1800), DER(90), PINC(90), RMINC(3,3,2)
      COMMON NINP, NOUT, TITLE, PAR,  RMINP, XZTHE, NS, NA, NPSI, INCEL,
     1  NPOT, NPRET, DELTE, ST, SS, XC, IPSI, IPCTR, IPSVEC, PARW,IPRET,
     2  ITCEL, RMAX, DMAX, DMAT, DINV, V1, V2, V3, V4, V5, A1, A2, A3,
     3  XTRAN, XMIN, XMAX, I, J, K, L, M, N, IS, IX, IA, IB, LTS,
     4  ITW, ISWIT, STWE, JTWE, LTSM, ITABW, LSS, C1, C2, C3, DIST,
     5  EZERO, ISEL, NC, XZPSI, XV, YV, PSINC, RTPSI, ITHE, JKTAB, DSTE,
     6  DER, PINC, GRAD2, SHIFT, KSTOP, NG, NTHE, E, RMINC, NPMAX
      DIMENSION NF(8), JF(8)
C     OUTPUT STWE TABLE FOR REFERENCE
   71 FORMAT(1HO 40H  TRANSLATIONS LISTED IN STWE TABLE      /1HO
     1           40H       LTS        X          Y          Z  /1H
     2  /(1H I10,3F10.2))
      WRITE OUTPUT TAPE NOUT, 71, (J,(STWE(I,J),I=1,3),J=1,LTSM)
    1 FORMAT(1HC 12H  DISTANCES F5.2,25H OR MORE LESS THAN DOJK  /1HO
     1  50H  IA   IB  LTS  LSS      DOJK       DOJK       DELTA /1H )
    2 FORMAT(1H 4I5,3F10.2)
    3 FORMAT(F10.2,F10.2,10I5,I2)
      READ INPUT TAPE NINP, 3, DLIST, BTEMP, (NF(I), JF(I), I=1, 5),
     1  ICARD
      WRITE OUTPUT TAPE NOUT, 1, DLIST
      DO 4  I=1, ITABW
      IA=JKTAB(1,I)
      IB=JKTAB(2,I)
      LTS=JKTAB(3,I)
      LSS=JKTAB(4,I)
```

```
      J=IPCTR(IA)
      K=IPCTR(IB)
      IP=IPREF(J,K)
      COJK=PAR(4*IP+28)
      CCJK=CSTE(2,I)
      IF (COJK-CCJK-CLIST)  4,6,6
    6 CELTA=CCJK-COJK
      WRITE OUTPUT TAPE NOUT, 2, IA, IB, LTS, LSS, COJK, CCJK, DELTA
    4 CONTINUE
   11 FORMAT(1HC 25H  INITIAL ROTATION MATRIX/1H (/1H 3F10.5))
   12 FORMAT(1HO 11H  XZTHE(1)=F6.2, 11H  XZTHE(2)=F6.2, 11H  XZTHE(3)=
     1  F6.2)
      CO 53  K=1, NTHE
      WRITE OUTPUT TAPE NOUT, 11, ((RMINP(I,J,K),J=1,3),I=1,3)
   53 WRITE OUTPUT TAPE NOUT, 12, (XZTHE(I,K),I=1,3)
   13 FORMAT(1HC 20H  LATTICE CONSTANTS 3F10.4,3F10.2)
      CO 14 I=28, 30
   14 PAR(I)=PAR(I)*57.29578
      WRITE OUTPUT TAPE NOUT, 13, (PAR(I),I=25,30)
   18 FORMAT(1HC 25H  POTENTIAL PARAMETERS   /1H (/1H 4F10.5))
      WRITE OUTPUT TAPE NOUT, 18, (PAR(I),I=31, NPMAX)
      IF (ICARD)  61, 61, 62
   32 FORMAT(14A5,A2)
   62 PUNCH 32,(TITLE(I),I=1,15)
   31 FORMAT(3F10.4,3F10.2)
      PUNCH 31, (PAR(I),I=25,30)
   34 FORMAT(4F10.5)
      PUNCH 34,(PAR(I),I=31,NPMAX)
   33 FORMAT(3F10.3,4I10)
      PUNCH 33, ((XC(J,I),J=1,3),ITHE(I),IPSI(I),IPCTR(I),I,I=1,NA)
   61 CONTINUE
C     LIST OF COORDINATES FOR THE ATOMS, HYBL LSSF FORMAT
   21 FORMAT(1HO 50H  ATOM          CARTESIAN                          CELL
     1       /1H  50H   IA       X          Y          Z          X
     2            15H Y          Z    /1H )
   22 FORMAT(1H I5,3F10.2,3F10.5)
      WRITE OUTPUT TAPE NOUT, 21
      CO 23  IA=1, NA
      CALL MV(DINV,XC(1,IA),V1)
      WRITE OUTPUT TAPE NOUT, 22, IA, (XC(I,IA),I=1,3), (V1(I),I=1,3)
   24 FORMAT(2H1C3F1C.5,F10.5,7X,3H1.0 7X,4H1.013X,1X,I5)
      IF (ICARD-2)  23, 63, 23
   63 PUNCH 24, (V1(I),I=1,3), BTEMP, IA
   23 CONTINUE
      RETURN
      END


     END       ACCNTA0C15  @D.WILLIAMS@                                  PCGC
     START     ACCNTA0C15  @D.WILLIAMS@                                  PCGC
     COMPILE   RUN  FORTRAN LIST                                         PCGC
C     SUBROUTINE PATCH(PARW)      SET DEPENDENT PARAMETERS
      SUBROUTINE PATCH(PARW)
      DIMENSION PARW(90)
      RETURN
      END


     END       ACCNTA0C15  @D.WILLIAMS@                                  PCGC
```